Co-Optimization of
Fuels & Engines

Multi-Mode: Gasoline Direct-Injection Sprays

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Project # ft074

2020 DOE Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

Overview: Gasoline Direct-Injection Sprays Multimode

Advanced Engine Development & Toolkit Development

Timeline

Task	FY16	FY17	FY18	FY19	FY20	FY21
		Phase 1		Phase 2		
E.1.4.2: SNL	Start		End	Re-Start		End
G.2.12: SNL			Start	End		
G.1.6: SNL					Start	End

Task	FY19	FY20
E.1.4.2: SNL Mixed mode: Fuel Effects on gasoline direct-injection sprays; Pickett, Skeen, Hwang, Sim, Yasutomi, Tagliante, Manin	$275k	$205k
G.2.12: SNL Quantify the impact of fuel properties on flash boiling to predict fuel spreading angle; Arienti, Wenzel.	$150k	
G.1.6: SNL Tip wetting for fuel blends & flash-boiling modeling; Arienti, Wenzel.		$200k

Barriers

- Need improved combustion modes & understanding of fuel effects thereon
- Understanding direct-injection sprays as a key pathway towards high-efficiency engines
  - Multimode & advanced compression ignition strategies have critical dependence upon injection control
- CFD model improvement for engine design/optimization

Partners

- Co-optima partners include nine national labs, one industry, 17 universities, external advisory board, and stakeholders (80+ organizations).
- 15 Industry partners in the AEC MOU.
- Task specific partners:
- Uses same hardware and operating conditions as Sandia engine (Sjöberg E.1.1.3)
- Engine Combustion Network, Spray G (20+ partners)
- Spray Combustion Consortium – Funds-in project
- Convergent Science Inc. – Software.
- + Many more – details in later slides

Relevance of fuel injection to advanced multimode combustion

Spray affects…

- liquid penetration, mixture preparation, and burn rate
- propensity to knock or auto-ignite in standard SI or multimode

Wall wetting or liquid in the bulk charge

- creates fuel-rich, PM-forming combustion
- slow vaporization is problematic even without wall impingement (dribble at end of injection)
- is not completely explained by fuel physical properties (distillation curve) or soot metrics (PMI index)

Conditions vary widely, significantly changing spray

Injection strategy for multimode combustion
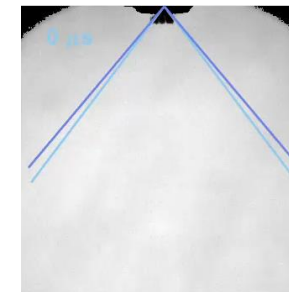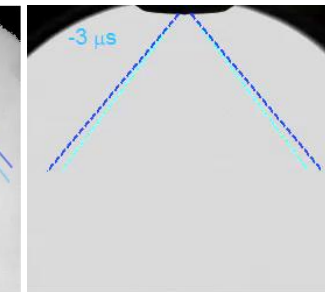
Sjöberg (Sandia)

Partial Fuel Stratified Lean

Crank Angle [°CA ATDC]
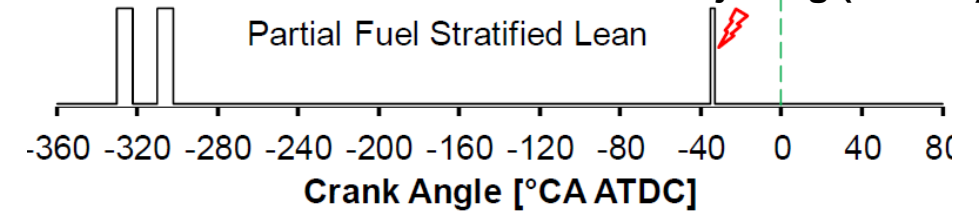
Intake injection (ECN* G3 condition)	Late injection (ECN G condition)	Near-TDC injection (High T, P condition)
333 K, 1.0 kg/m³	573 K, 3.5 kg/m³	800 K, 9.0 kg/m³
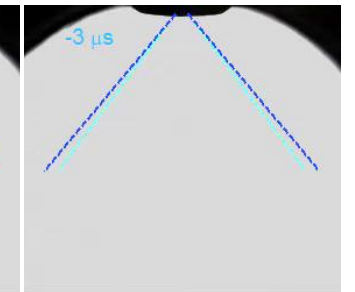
With intake T=333K, P=1.0bar, CR=12

CAD TDC	Temperature	Pressure	Density
intake open	333 K	1.0 bar	1.1 kg/m³
-52	511 K	5.2 bar	3.6 kg/m³
-19	711 K	18.7 bar	9.2 kg/m³

- Multimode operation involves mixture preparation and combustion in a "beyond-RON" regime compared to conventional SI (along with overall fuel-lean conditions)
- What fuel is preferred for this regime?
  - Multimode (Mazda SPCCI) tolerates lower octane (80 AKI) gasoline[1,2] but is it "ideal"?
  - Reference CoOptima investigations:
    - Szybist (FT069, 2019) shows significant LTHR and sensitivity/octane index effects in beyond-RON space
    - Sjöberg (FT070, 2019) suggests best operation using high RON and high sensitivity fuels
- We consider mixture preparation, spark (laser)-ignition, and auto-ignition in highly stratified (mixture and temperature) spray mixtures
  - Autoignition and LTHR visualization using optical and laser diagnostics, specifically for PRF80-PRF100 fuels in beyond-RON space
  - Autognition experiments not reviewed here because of time limitations

Injection strategy for multimode combustion

Sjöberg (Sandia)

Partial Fuel Stratified Lean

Crank Angle [°CA ATDC]

Regime of spray mixing, spark ignition, flame, autoignition?

Fuel injection

Beyond RON

Mazda SPCCI multimode
CR = 16.3
supercharged
(+ Miller cycle)

P_{in} = 2.0 bar

CR = 16

1.5 bar

1.0 bar

CR = 12 (solid)

P_{in} = 0.5 bar

Beyond MON

Pressure [bar]

Temperature [K]

1. https://www.autoblog.com/2018/01/25/mazda-skyactivx-compression-ignition-explained/
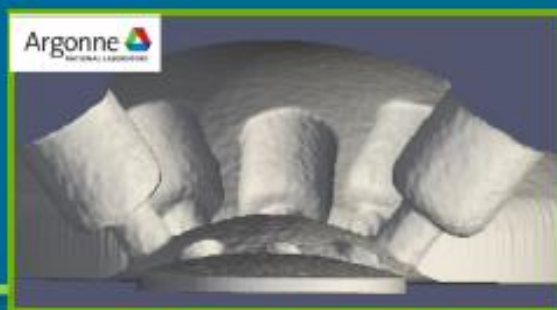2. https://www.roadandtrack.com/car-culture/a17171105/mazda-skyactiv-x-how-it-works/

Overall technical approach

**E.1.4.2: Experiment
Liquid position / mixing measurement
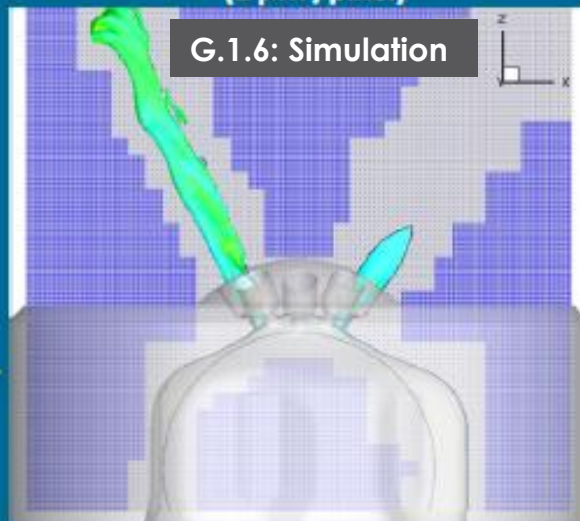(Chamber funded by past Co-Optima work)**

Coupled level-set VOF simulation `G.1.6: Simulation`
& homogenous relaxation modeling (CONVERGE) `G.2.12`

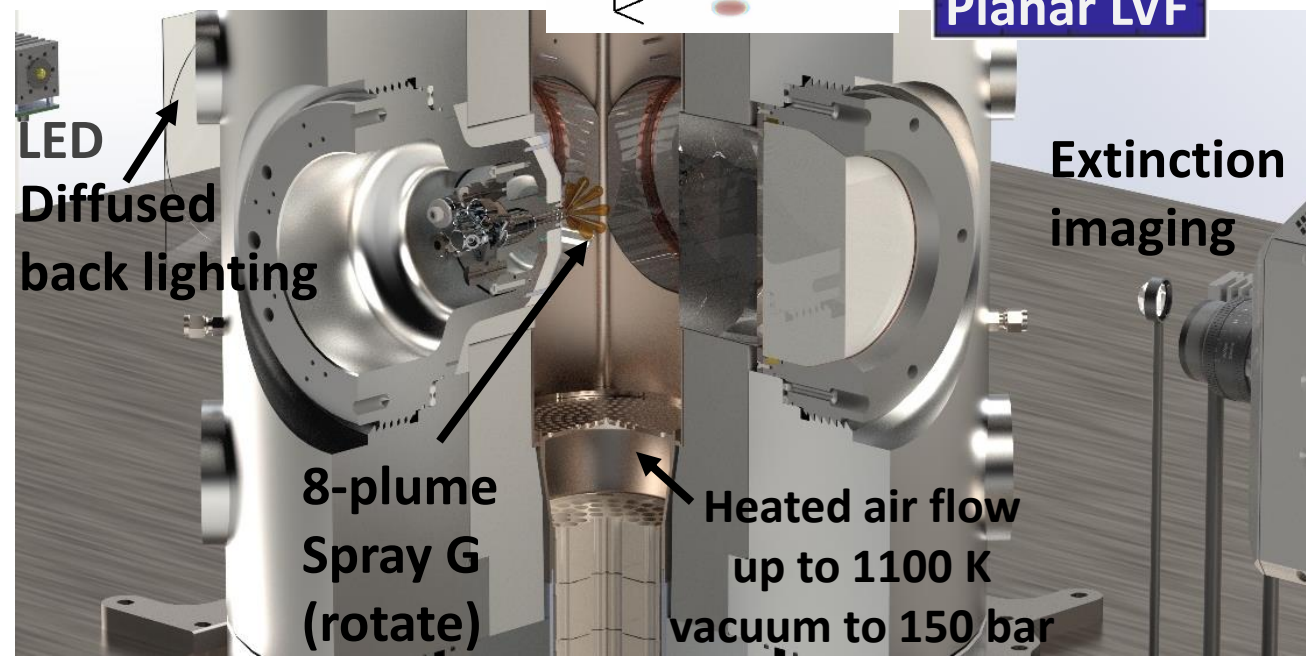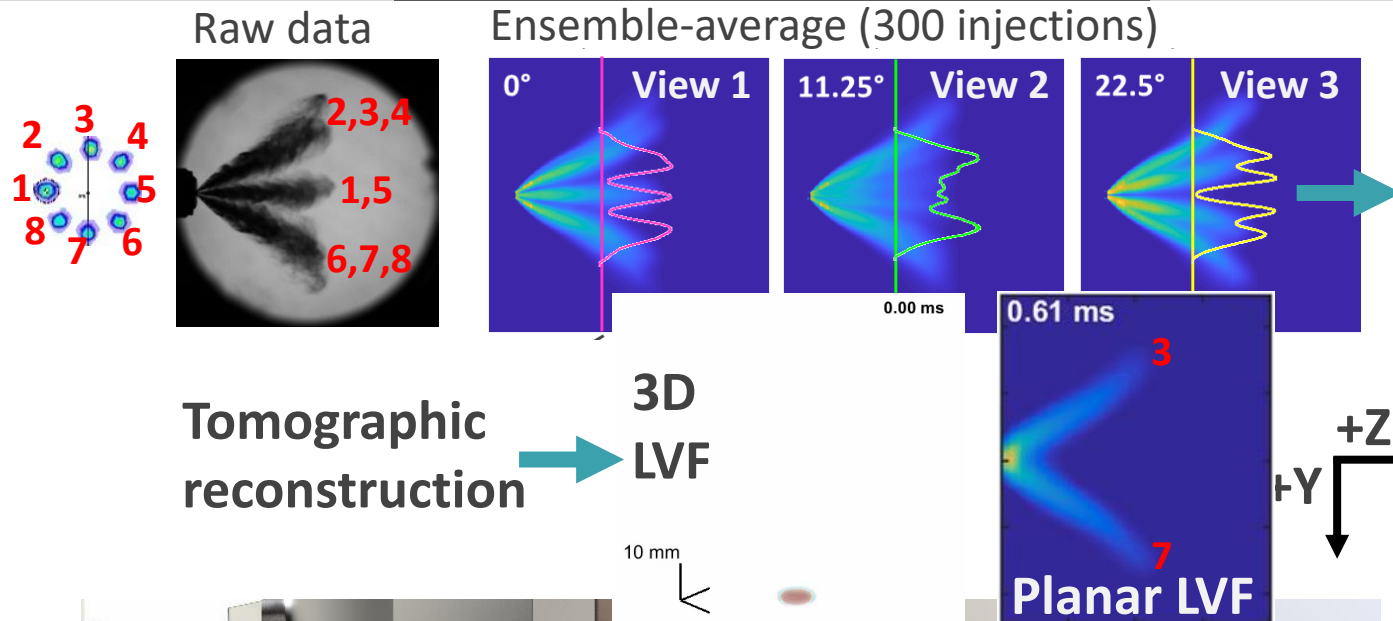Injector surfaces are reconstructed from X ray radiography and converted into a computational mesh

Argonne NATIONAL LABORATORY

High-precision scanning (1 μm /pixel)

Computational domain

`G.1.6: Simulation`

CLSVOF ongoing simulation with embedded boundary

Raw data

Ensemble-average (300 injections)

2 3 4
1 5
8 7 6

2,3,4
1,5
6,7,8

0° View 1   11.25° View 2   22.5° View 3

Tomographic reconstruction → **3D LVF**

0.00 ms   0.61 ms

3
7

Planar LVF

+Z
+Y

10 mm

LED Diffused back lighting

8-plume Spray G (rotate)

Heated air flow up to 1100 K vacuum to 150 bar

Extinction imaging

Setup for laser ignition, with OH* and extinction

OH*
Focused laser beam for ignition
Intensifier
Diffused lighting
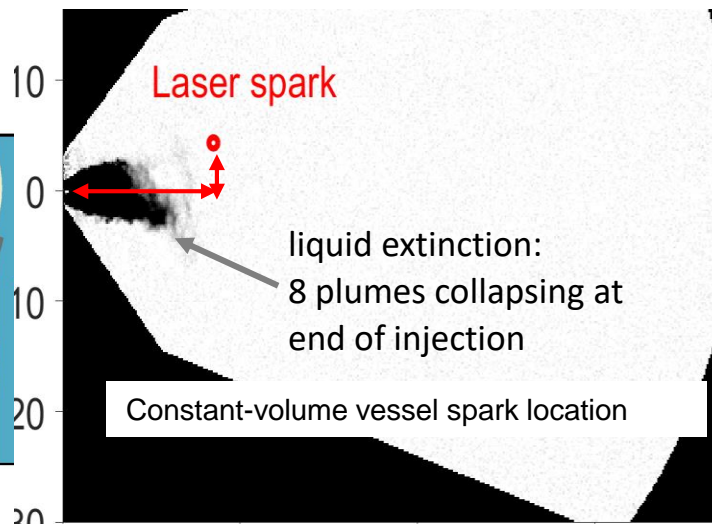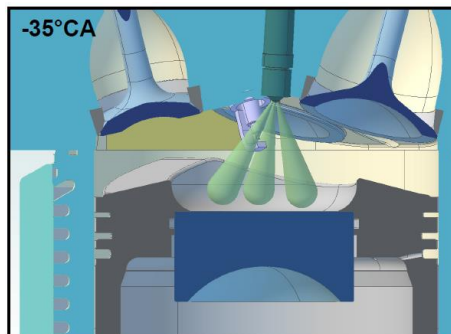Extinction and chemiluminescnece
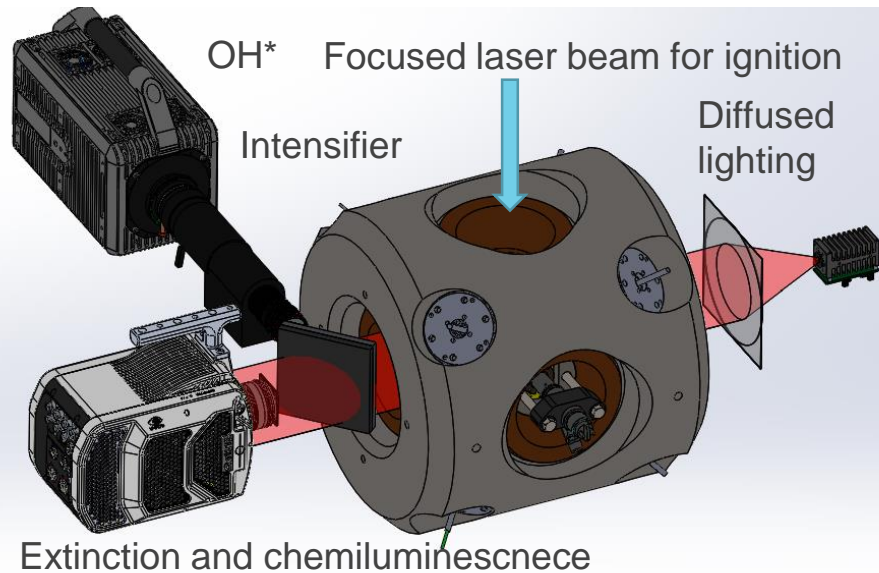
- Study stratified autoignition of single- and multi-hole fuel injectors, using a range of fuels
- Apply advanced optical diagnostics to detect ignition and cool flame (e.g. formaldehyde)
- Simultaneously measure flame position and liquid or soot extinction, indicating sources of imperfect mixing
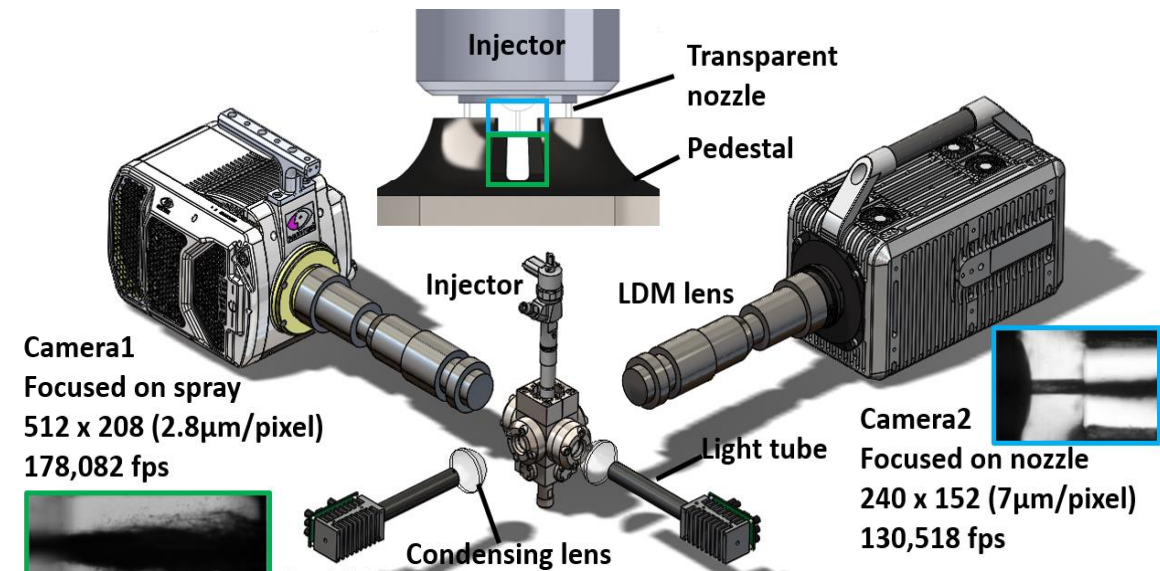- CFD (CONVERGE) simulations applied to provide estimates for mixture (equivalence ratio) evolution

E.1.4.2

Using SIDI 8-hole injector, apply laser spark ignition

Sjöberg (Sandia)
E.1.1.3 task

-35°CA

Laser spark

liquid extinction:
8 plumes collapsing at end of injection

Constant-volume vessel spark location

Injector
Transparent nozzle
Pedestal
Injector
LDM lens
Camera1
Focused on spray
512 x 208 (2.8µm/pixel)
178,082 fps
Light tube
Camera2
Focused on nozzle
240 x 152 (7µm/pixel)
130,518 fps
Condensing lens

- Visualize internal flow and emerging spray for single-hole GDI at flash-boiling conditions; data used for

G.2.12

Fuels considered

| Parameters	iso-octane	di-isobutylene	olefinic	e30
Density @15°C [kg/m^3]	698.7	736.2	722.9	752.7
Viscosity (ν) @40°C [mm^2/s]	0.574	0.541	0.477	0.695
Viscosity (μ) @40°C [10^{-3}Pa·s]	0.401	0.398	0.345	0.523
Research octane number (RON)	100	98.3	98.3	97.9
Motor octane number (MON)	100	88.5	87.9	87.1
Vapor pressure @90°C [kPa]	70.9	74.2	170.6	286.8
Aromatics (vol.%)	0	20.1	13.4	8.1
Olefins (vol.%)	0	4.0	26.5	5.0
Paraffins (vol. %)	100	56.3	56.4	57.1
Cycloalkanes (vol. %)	0.0	0.0	2.9	7.0
Ethanol (vol. %)	0.0	0.0	0.0	30.0
Lower heating value [MJ/kg]	44.8	43.5	44.1	38.2
Stoichiometric A/F ratio [-]	15.1	14.7	14.8	12.8
Heat of vaporization [kJ/kg]	20.8	21.5	21.1	38.4

- **iso-octane: single component, flat distillation temperature**
- **di-isobutylene: multi-component (5), narrow-range distillate**
- **olefinic: multi-component, wide-range distillate**
- **e30: multi-component, wide-range distillate, with 30% ethanol**
- **E00: 3 component non-reacting surrogate: 0.36 n-pentane, 0.46 iso-octane, 0.18 n-undecane**
- **PRF80: for studies of autoignition with a lower octane number**
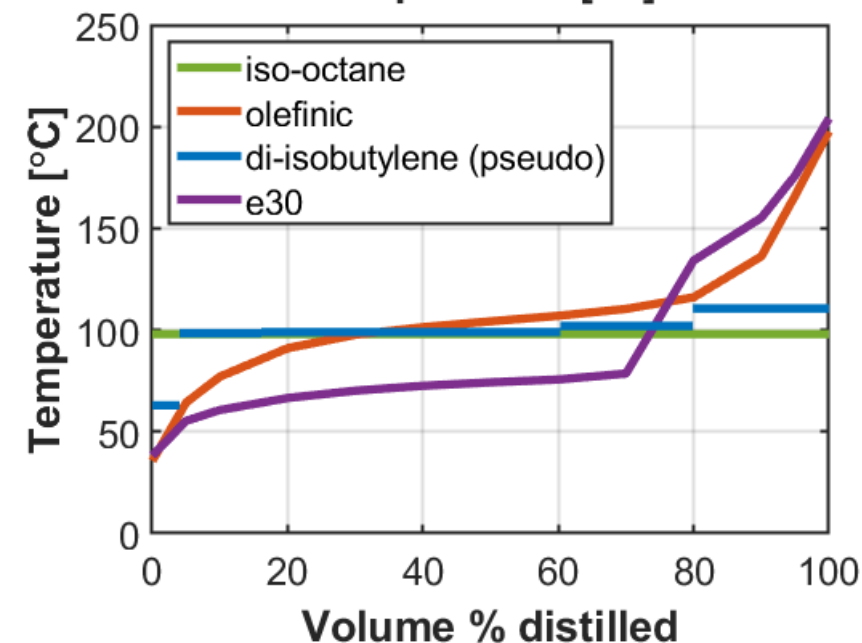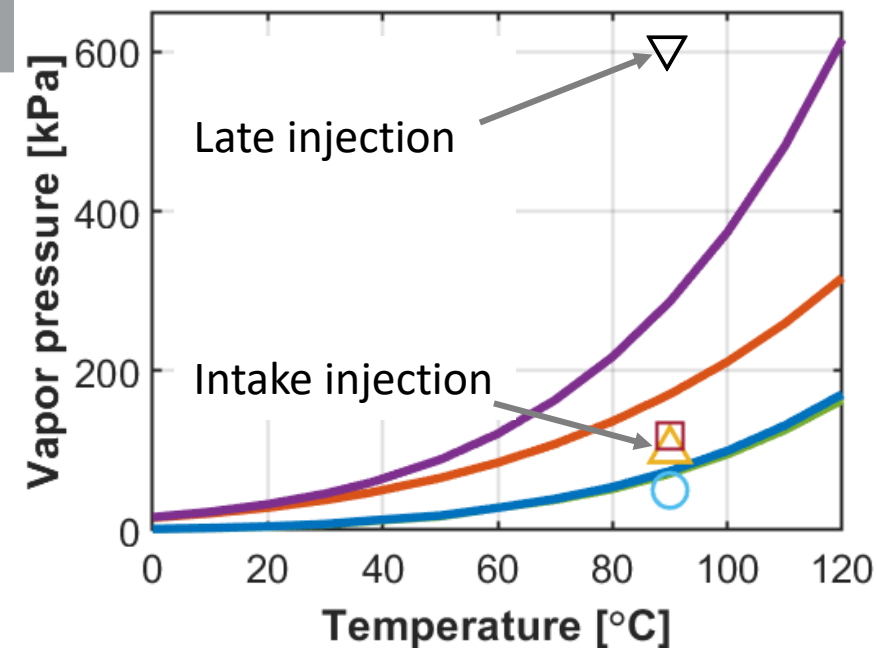
HRM model:

$$\frac{Dx}{Dt} = -\frac{x - \bar{x}}{\Theta_{HRM}}$$

Vapor quality:
$$x = \frac{\frac{1}{\rho_{L,sat}} - \frac{1}{\rho_{mix}}}{\frac{1}{\rho_{L,sat}} - \frac{1}{\rho_{V,sat}}}$$
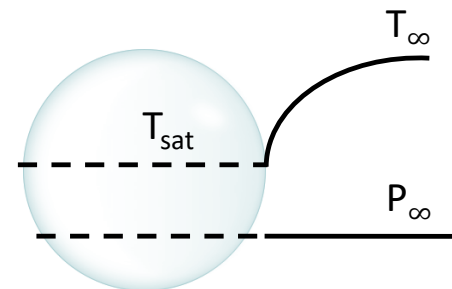
Equilibrium value:
$$\bar{x} = \frac{h - h_l}{h_v - h_l}$$

G.2.12

New bubble submodel:

- Controlled by diffusion to bubble surface
- Gradients in temperature and bubble growth considered
- Properties of hydrocarbon fuels considered, rather than using relations developed for water/steam system
- Implemented as a user function within CONVERGE CFD

$$\bar{T}_L(t) = \frac{3}{R_{max}^3 - r_b(t)^3} \int_{r_b(t)}^{R_{max}} r^2 T_L(r) dr$$

Old HRM model:

$$\Theta_{HRM} = 3.84 \cdot 10^{-7} \phi_0^a \psi^b$$

$$\psi = \left| \frac{P_{sat} - P}{P_{crit} - P_{sat}} \right|$$

$$\phi_0 = \frac{\frac{m_g}{\rho_g}}{\frac{m_g}{\rho_g} + \frac{m_l}{\rho_l}} \frac{n_{vap}}{n_{vap} + n_{NC}}$$

$$Jac = \frac{\rho_{vap}}{\rho_{liq}} \frac{c_{p,liq}}{h_{vap}} \frac{\Delta T_0}{h_{vap}}$$
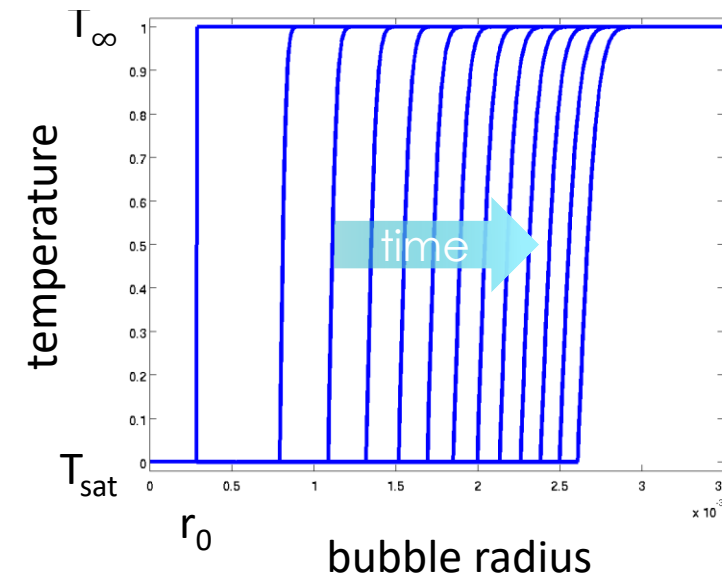
Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
Sept 2019, SNL E.1.4.2	Provide initial database for multimode ignition in stratified mixtures for comparison to ignition characteristics of homogenously/mixed and compressed ignition (tracked)	**complete**
March 2020, SNL G.1.6	Completed film-tracking simulations to quantify end-of-injection dribbling and tip wetting (tracked)	**complete**
Sept 2020, SNL E.1.4.2	Provide quantitative equivalence ratio measurements for fuels/injectors/injection durations (tracked)	**on track, per COVID19-delay**
Sept 2020, SNL G.1.6	Develop droplet evaporation within VOF simulations.	**in progress**
Aug 2019, SNL E.1.4.2	Provided spray measurements for LNF injector used for ANL (G.1.10 & G.2.1) & ORNL (Edwards) simulations	**complete**
Aug 2020, SNL G.1.6	Peform simulations using improved HRM model at Spray G2 conditions	**in progress**

Technical Accomplishments Summary

Experiments

- Liquid distribution measurements at conditions of multimode, late injection for various fuels

- Transparent nozzle and near-injector plume growth experiments at flash boiling conditions

- Laser-ignition in stratified spray conditions with unique flame and quantitative soot extinction measurement, demonstrating requirements to reach soot-free combustion

- Autoignition experiments in PRF80 fuel sprays demonstrate a potential role of cool-flame radical transport on ignition and combustion

Simulations & Modeling

- Implementation of new HRM-Thermo model to account for local temperature and bubble radius under flash-boiling conditions

- CLSVOF simulations
  - Spray G ECN cond. (steady state): iso-octane & BOB4
  - Spray G ECN cond. (end of inj.): iso-octane

- CONVERGE simulations
  - Simulations in comparison to experiment over a range of saturated pressure ratio for single-axial nozzles
  - ECN G2 condition
  - Simulations of multi-hole GDI mixing at laser-ignition conditions
  - RANS combustion simulations, identifying an overestimate in turbulent combustion speed (E.1.4.2)

Plume direction angle at Z=30 mm

Early injection conditions: 0.5 bar "G2"

- **3D measurements of plume direction coupled to vapor boundary from schlieren measurements**

Plume direction angle

Orifice outlet

α

2·α=cone angle

Averaged plume center

Point on vapor boundary

Vapor boundary with intermittency of 0.5
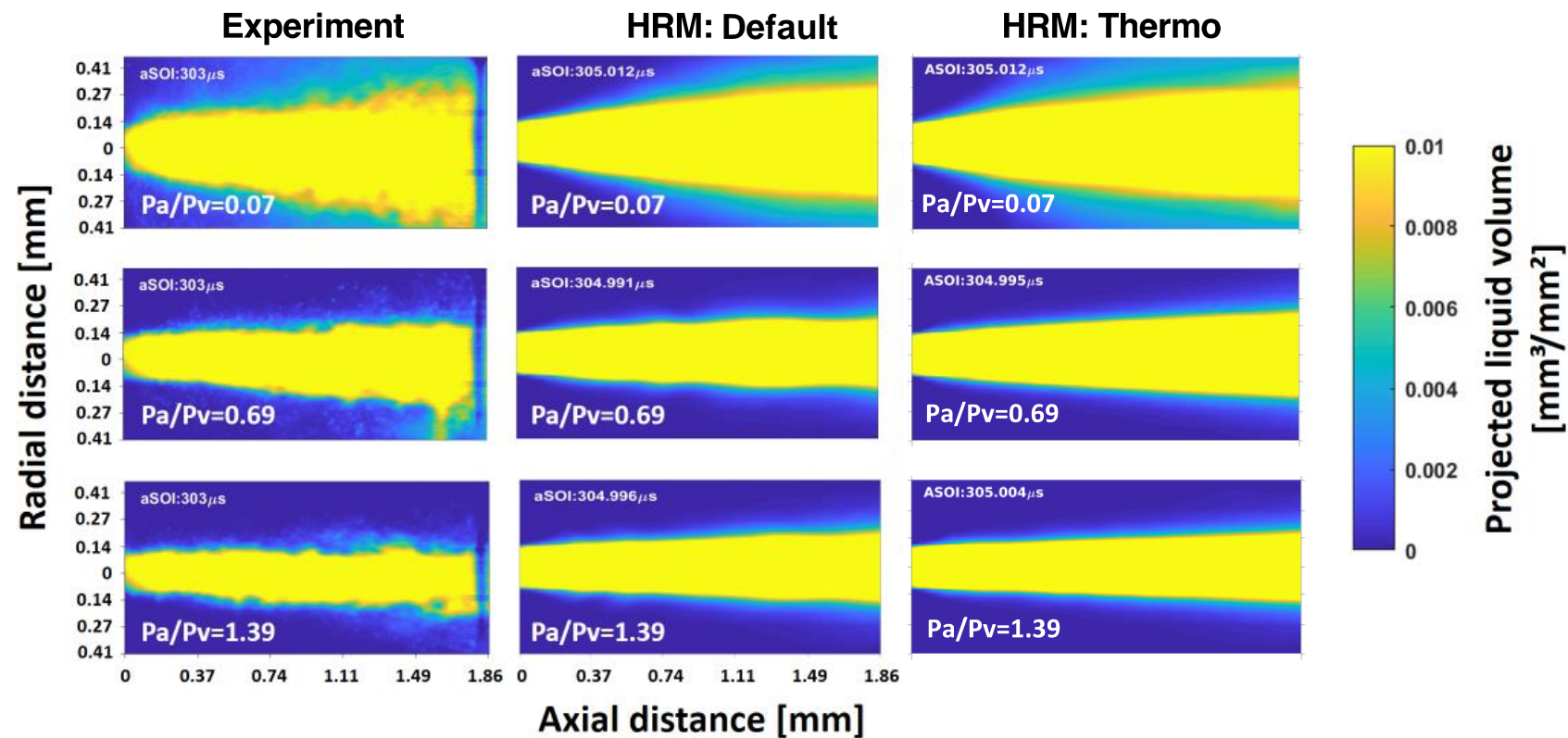
Projected liquid volume [mm³/mm²]:

$$\tau \frac{\pi \, d^3/6}{C_{ext}} = \int_{-y_\infty}^{y_\infty} LVF \cdot dy$$

LVF: liquid volume fraction
d: droplet diameter
C_{ext}: extinction cross-section from Mie-theory
τ: optical thickness

Experiments supported by Spray Combustion Consortium
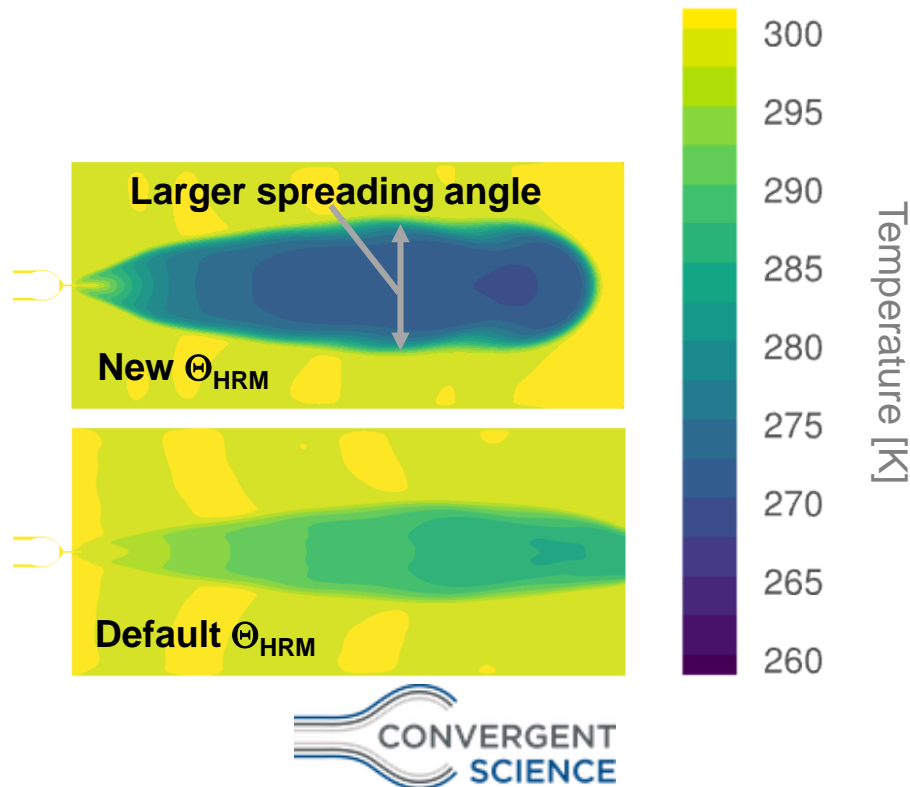SAE paper 2020-01-0828 analysis and writing supported by E.1.4.2
Manuscript submitted to IJHMT supported by G.2.12

G.2.12+E.1.4.2: New HRM model shows more vaporization cooling and better predictions of boil-off after end of injection
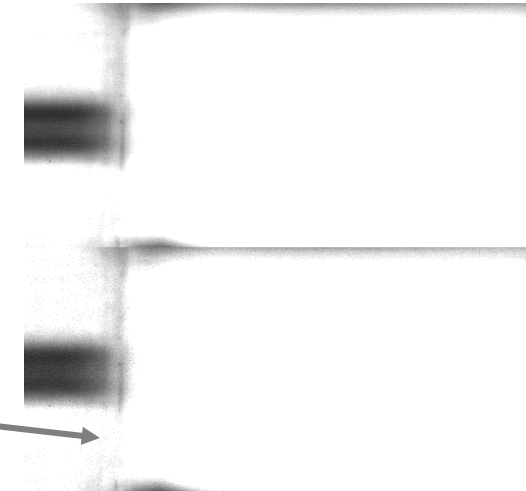
ACCOMPLISHMENTS (2/12)

- **3D measurements of plume direction coupled to vapor boundary from schlieren measurements**
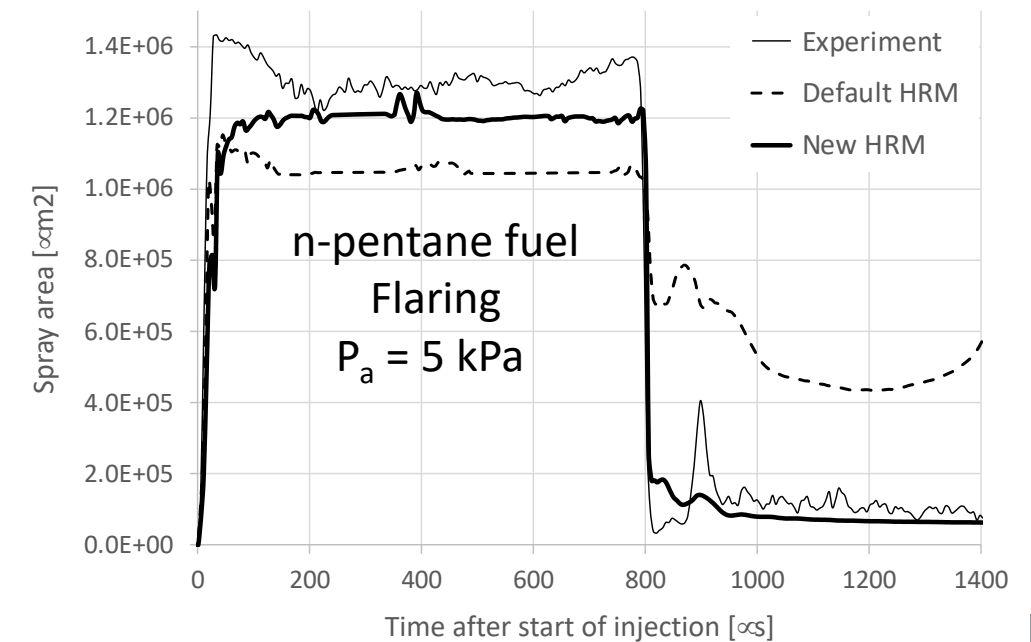
non-flashing
$P_a/P_{vap} = 1.3$

film forms during injection—possible only with cooling
Tsat(20 kPa) = 270 K

flash-boiling
$P_a/P_{vap} = 0.3$

Larger spreading angle

New Θ_{HRM}

Default Θ_{HRM}

Temperature [K]

300
295
290
285
280
275
270
265
260

CONVERGENT SCIENCE

Experiment
Default HRM
New HRM

n-pentane fuel
Flaring
$P_a = 5$ kPa

Spray area [∝m2]

1.4E+06
1.2E+06
1.0E+06
8.0E+05
6.0E+05
4.0E+05
2.0E+05
0.0E+00

0   200   400   600   800   1000 1200 1400

Time after start of injection [∝s]
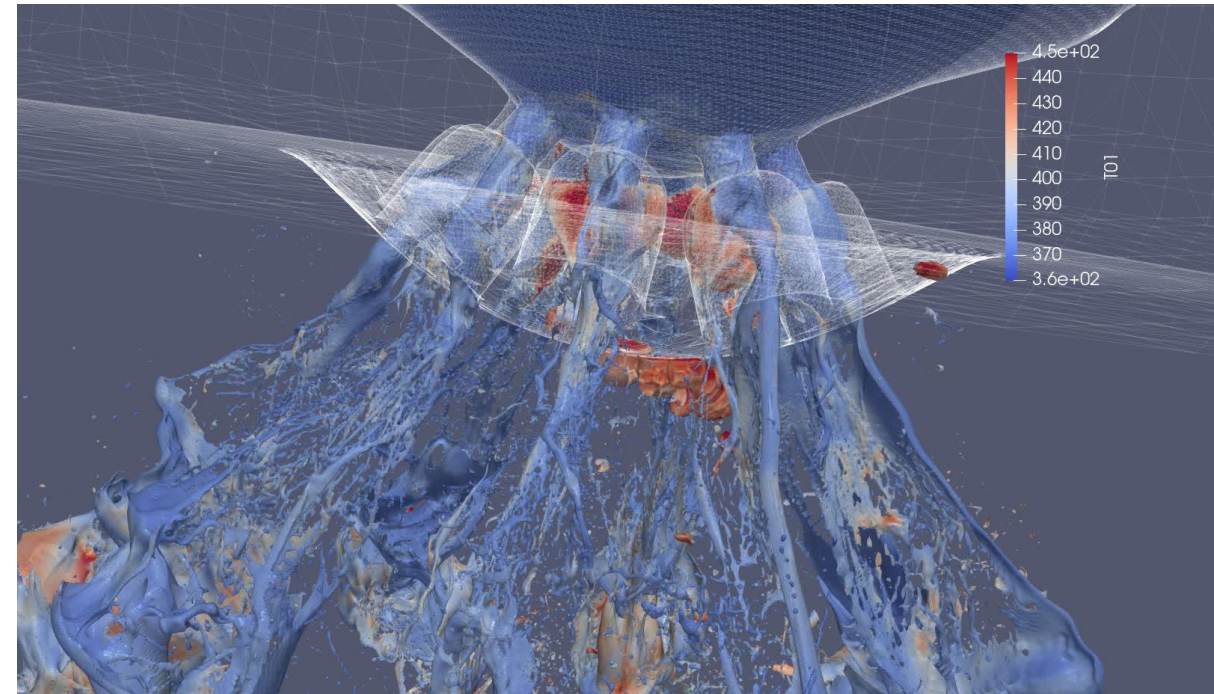
- **Simulations for single-component fuel build the foundation in capability to understand fuel effects on film formation, affecting soot and deposit formation**
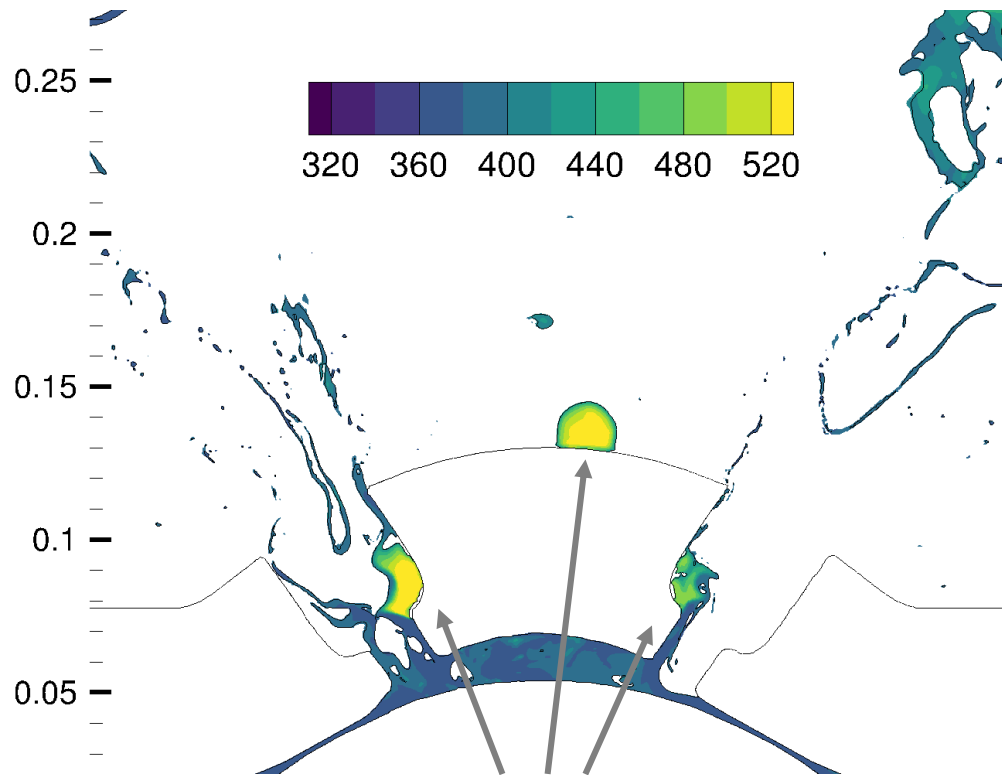
Film deposits inside counterbore and on face of injector

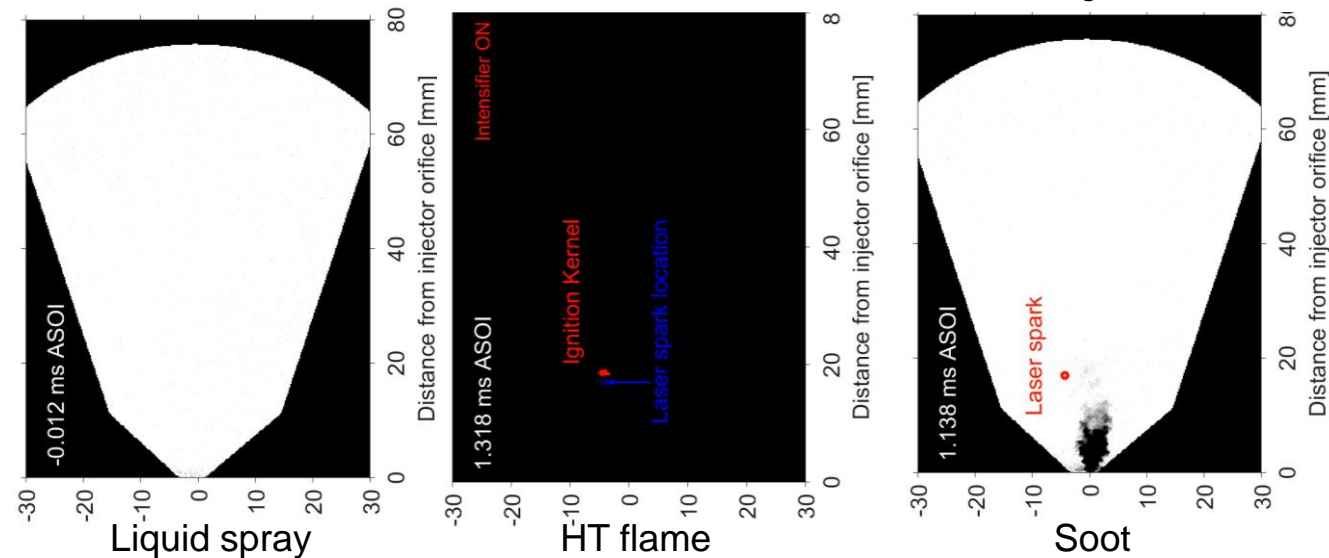CLSVOF simulation of Spray G using iso-octane fuel. Needle during closing with a lift of 11 μm.

- **Increasing delay of laser ignition after the end of injection significantly decreased soot formation, with a slight increase in combustion efficiency due to rapid flame propagation through the stratified fuel mixture downstream**

- **The experimental results are used as a database for the numerical simulation, which will provide qualitative measurement of the mixing**

Fuel	iso-octane
Ambient P [bar]	36.8
Ambient T [K]	850
Amb. density [kg/m³]	15.0
Oxygen [mol%]	21

LI 0.07 ms after the end of injection
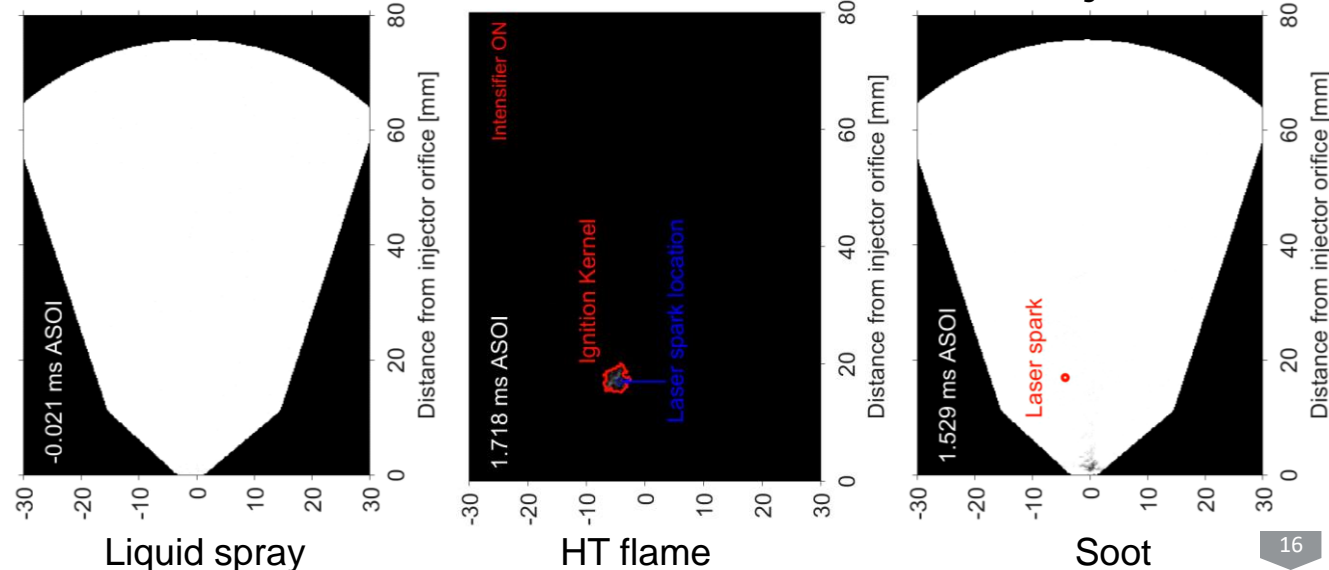
Liquid spray   HT flame   Soot

LI 0.45 ms after the end of injection

Liquid spray   HT flame   Soot

RANS CFD of spray mixing
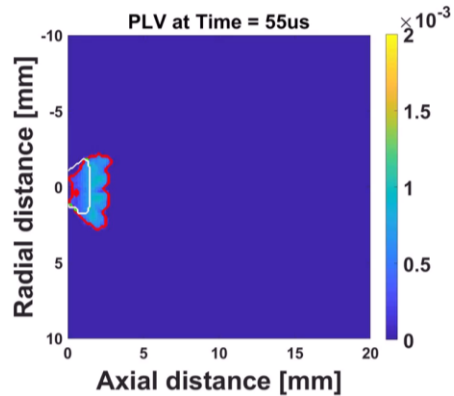
Flame tracking defines volume of interest for mixture

OH* chemiluminescence Experiments

Control cube

$$\Phi \to m_{IC_8H_{18}}$$
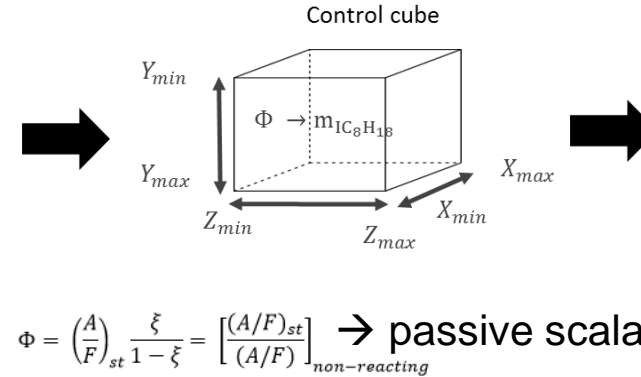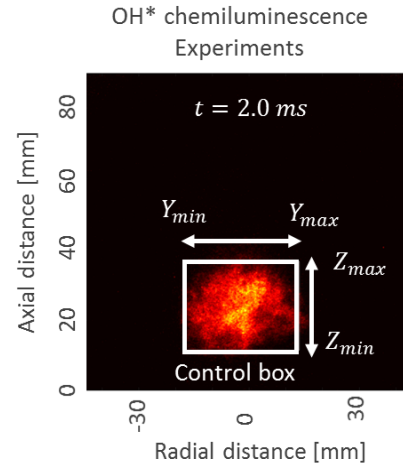
$$\Phi = \left(\frac{A}{F}\right)_{st} \frac{\xi}{1-\xi} = \left[\frac{(A/F)_{st}}{(A/F)}\right]_{non-reacting} \to \text{passive scalar}$$

NON-reactive RANS

$t = 2.0\ ms$

$Y_{C_8H_{18}}$
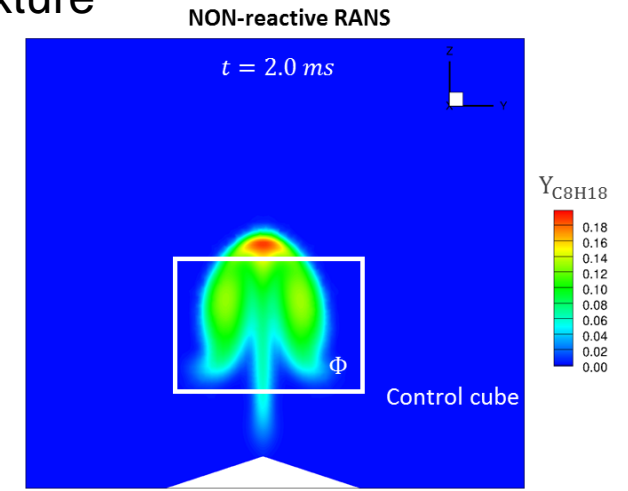
After laser ignition the fuel mass is computed for a range of equivalence ratios (Φ) in the control cube (following the **flame** based on the experiments) for each timing

Early laser ignition (0.52 ms after the end of injection)

Soot

Φ > 2
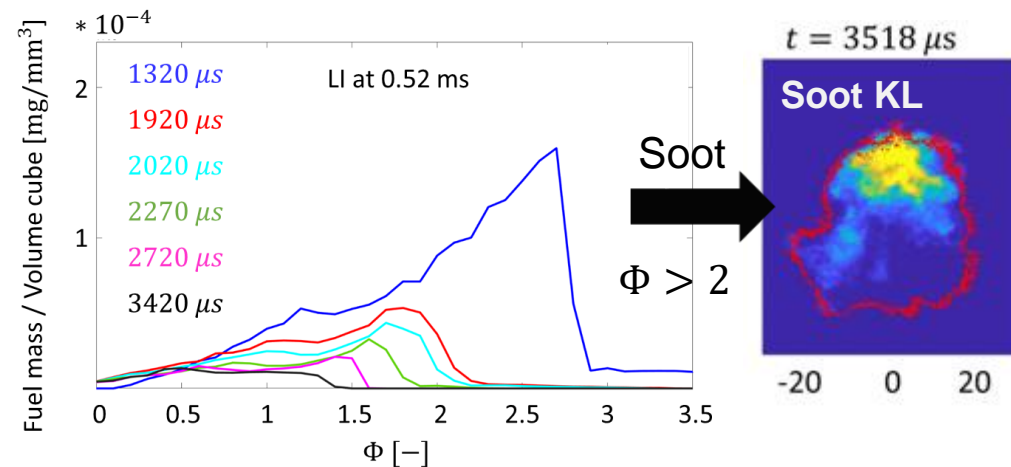
Late laser ignition (1.92 ms after the end of injection)

Soot free

The flame never propagates in regions where Φ > 2

Soot from dribble is always observed!

Comparison OH* Expe / OH Converge at 1720us
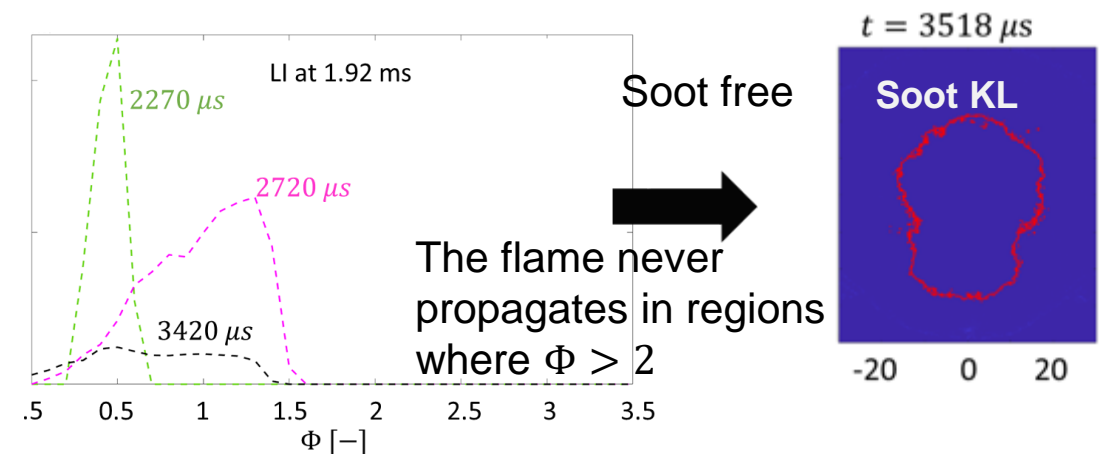
Green iso-line: RANS Y_{OH} projection

RANS

Experiment

Pressure rise [kPa]

Time ASOI [ms]
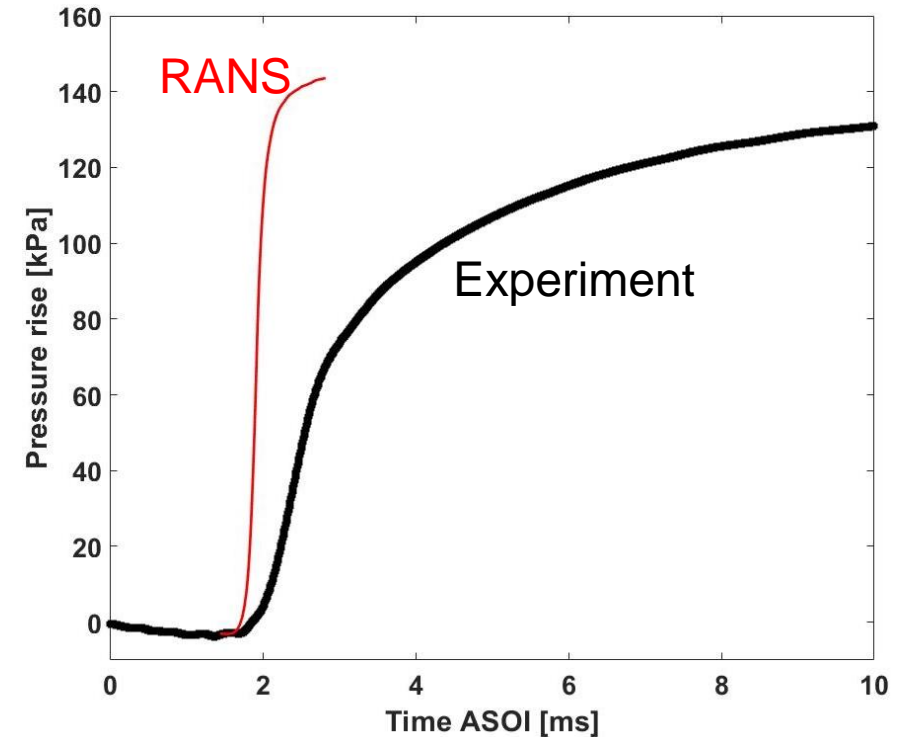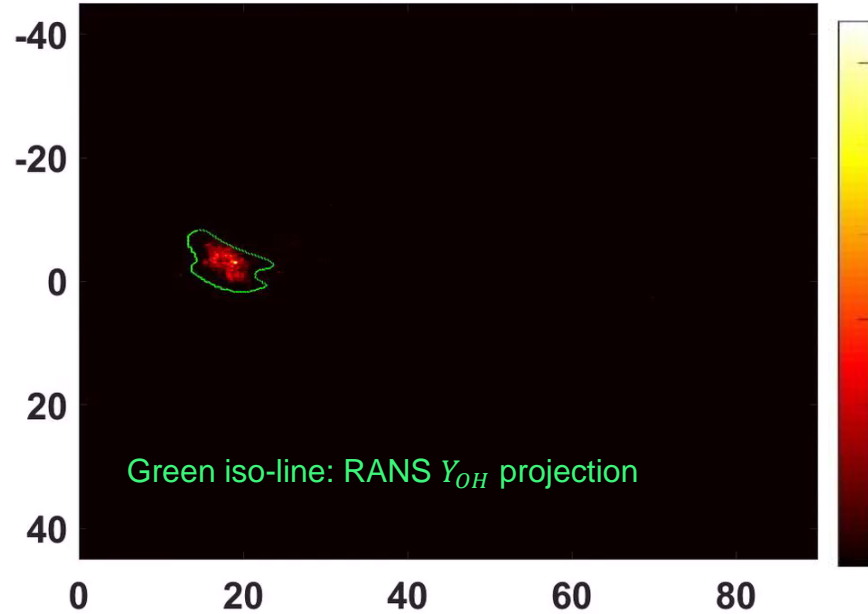
Simulations have been performed varying the chemical mechanism, ignition location, and timing. They all present the same characteristics:

- The flame propagates too fast, especially at the jet periphery

- Turbulent flame speed functions follow $S_T = S_L\sqrt{\mu_t/u}$. Predicted μ_t/u <u>exceeds 1500 </u>in the wake of the highly turbulent injection, which affects G equation flame speed or direct well-stirred reactor combustion model (SAGE).

Responses to Previous Year Reviewers' Comments

Overall Approach:

Reviews positive from all reviewers. G.1.6: Suggested inclusion of open-source code to allow VOF simulation tool to be used by industry and academia. Response: We appreciate the positive feedback. We have included more conventional codes such as CONVERGE CFD in this work to have greater reach.

Accomplishments:

A reviewer noted "measurement of key elements in sprays is advanced while CFD of the model is not enough to support the physics found in the experiment." Response: it will take time to reach the range of conditions explored in the experiment but the foundation is being laid… .

Collaboration and Coordination:

Reviewers noted "Excellent collaboration" and "more coordination between experiment and simulations". Response: coordination is active but expectations on the range of operating conditions need to be adjusted based on the complexity of the calculation method. We have included clear joint experiments and simulation during this FY and plan to continue.

Proposed Future Research:

Reviewers said "future plans include the desirable improvements in each area" and "suggested continuing to work on CFD model improvement and seeing the 3-D liquid volume fraction for the asymmetric multi-hole spray injection". Response: We have characterized side-hole injection equipment in this FY, and invented a way to perform computed tomography with many rotation views automatically.

Relevance—Does this project support the overall DOE objectives?

Very positive feedback on this question from all three reviewers: "it supports the Co-Optima goals" and "is well-aligned with DOE objectives," Response: We appreciate the positive feedback.

Collaboration and Coordination with Other Institutions

- **E.1.4.2 Project collaborators include (still just a partial list):**
  - Sandia: Sjöberg using same injector as E.1.1.3 task and coordinating closely on operating conditions, results, and fuels. Data supports G.1.6. Data also supports CFD efforts for DOE PACE project by J. Chen and T. Nguyen.
  - Argonne: Powell applies x-ray diagnostics for Spray G at similar operating conditions, leading to understanding about plume growth
  - Provide injector measurements to other Co-Optima projects at ANL (G.1.10 & G.2.1) & ORNL (Edwards) for CFD simulations
  - Engine Combustion Network data posted online at ecn.sandia.gov, where 20+ experimentalists and users apply this data to guide experiment and CFD simulations
  - Erlangen Univ: Weiss (Wensing group) visited Sandia and collaborated on the development of the computed tomography method, permitting the 3D measurement of liquid distribution
  - City Univ: Karathanissis and Koukouvinis (Gavaises group) visited Sandia and participated in 3D CT with other gasolines and transparent nozzle experiments

- **G.1.6: Project collaborators include:**
  - multiple investigators (~15) perform experiments and simulate the Spray G internal and external conditions used in these studies
  - Prof. Mark Sussman, Florida State Univ.: Development & testing of numerical methods for fuel inj. applications
  - Center for Computational Sciences & Engineering, Berkeley Lab: Development of library for hierarchical adaptive mesh refinement in high-performance computing

Remaining Challenges and Barriers

- **E.1.4.2 spray experiments:**
  - Quantitative vapor mixture fraction measurements in the midst of liquid droplets and dribble
  - Providing meaningful and unique data while also performing fuel variations, that include multi-component fuels with a wide distillation curve and differential evaporation effects
  - Expansion of autoignition operating conditions and fuels

- **G.1.6 modeling and simulations:**
  - Implementation of more detailed computational models for cavitation and flash-boiling, in relation to the operation mode of modern injectors.

- **E.1.4.2 spray experiments:**
  - Determine if advanced hardware (high injection pressure GDI) can alter mixtures, dribble, and ignition characteristics
  - Consider fuels specifically used for compression ignition, including diesel- and gasoline-range CoOptima blends. Work thus far has provided foundational understanding but has not explored the full range of potential fuels
  - The experiments planned will establish if fuel physical properties can directly lead to mixtures that are more or less rich at similar delays after the start of injection, providing means for changing equivalence ratio distribution or avoiding soot formation
  - Demonstrate how distillation shape needs to be altered to mitigate liner impingement

- **G.1.6 modeling and simulations:**
  - CLSVOF: Apply validated simulation capability to evaluate the role of fuel blend composition (e.g., light vs. heavy components) in differential evaporation
  - Develop an efficient model to rank fuel blends by propensity to form soot from fuel deposits in he film boiling regime
  - CONVERGE: Validate new flash-boiling relaxation model with USAXS (ANL) data for 80% iso-octane 20% BuOH and 80% iso-octane 20% EtOH
  - Analyze plume collapse at flash-boiling conditions as a function of ethanol content

Summary

Experiments

- 3D liquid volume fraction measurements show a strong effect of fuel type during intake injection, but less difference at late-injection conditions

- Plume direction and collapse is strongly dependent upon local plume cone angle, with dependence upon fuel and operating conditions

- Transparent nozzle experiments at flash-boiling conditions show effect of pressure ratio on plume growth, but also on evacuation of the sac after the end of injection

- Laser ignition in stratified mixtures can be timed to avoid soot formation, but soot from dribble sources near the injector remains problematic

- Autoignition experiments in PRF80 fuel sprays also demonstrate soot-free combustion.

- PRF80 schlieren and high-speed LIF diagnostics demonstrate a potential role of cool-flame radical transport on ignition and combustion at multi-mode conditions

Simulations & Modeling

- Implementation of new HRM-Thermo model shows distinct improvement in plume growth, temperature deficit, and evacuation of the sac to account for local temperature and bubble radius growth under flash-boiling conditions

- Liquid structure and wetted surfaces are predicted using CLSVOF interface tracking during end of injection periods

- RANS combustion simulations show excessive flame speed and heat-release rates with high turbulence generated by the spray (E.2.1.4)
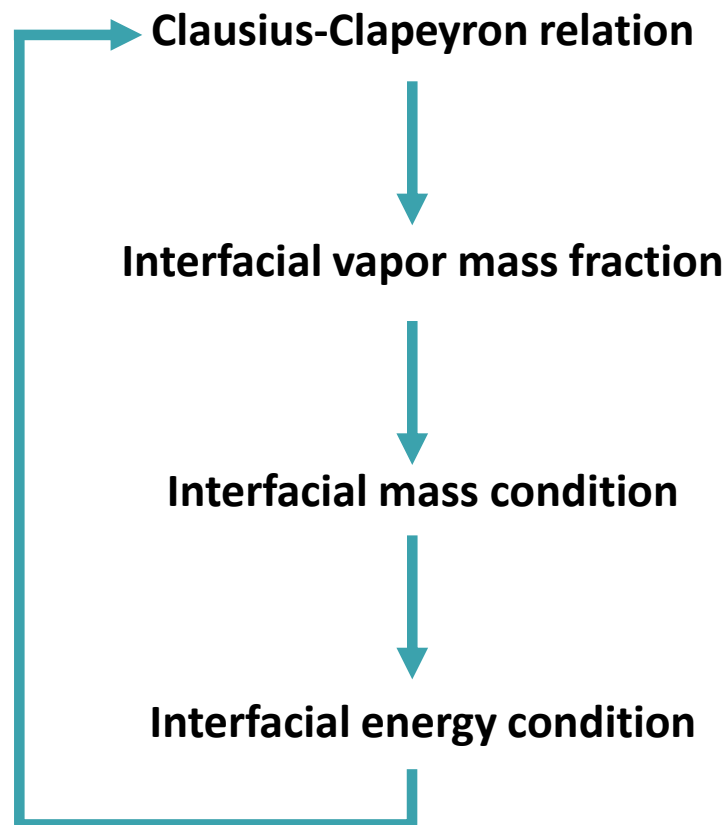
Technical Back-Up Slides

- Novel approach for compressible flow in sharp-interface method (CLSVOF)
- Exact determination of interface temperature through iterative solution
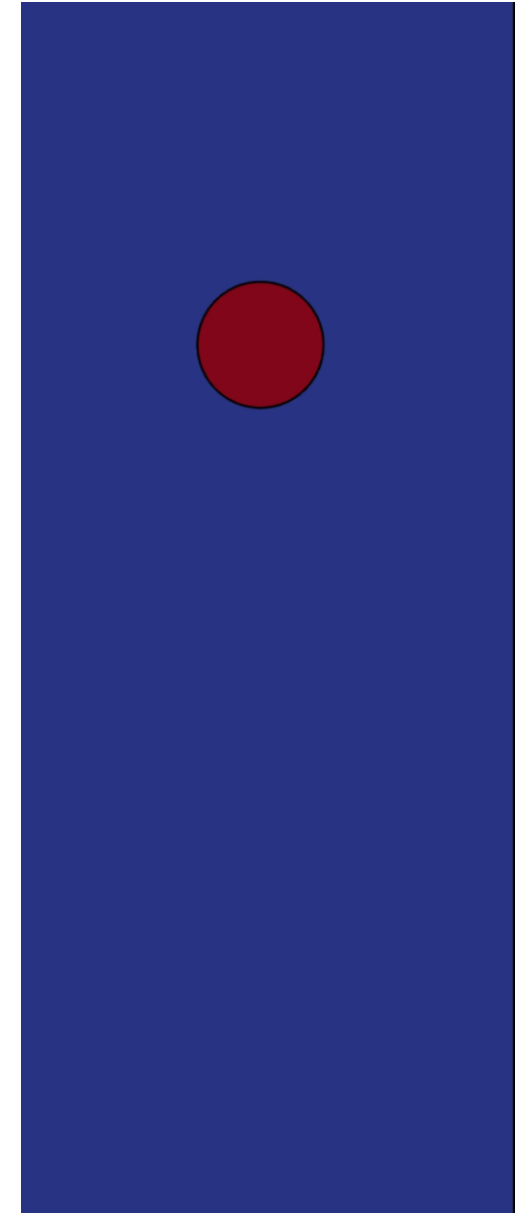- Consistent evaluation of gradients in mass fraction and temperature

Clausius-Clapeyron relation

$$X = \exp\left[-\frac{L_v M_v}{R}\left(\frac{1}{T_\Gamma} - \frac{1}{T_{\text{sat}}}\right)\right]$$

Interfacial vapor mass fraction

$$Y = \frac{X M_v}{X M_v + (1 - X) M_g}$$

Interfacial mass condition

$$\dot{m} = \frac{\mathbf{n}_\Gamma \cdot \rho_g D \nabla Y}{Y_\Gamma - 1}$$

Interfacial energy condition

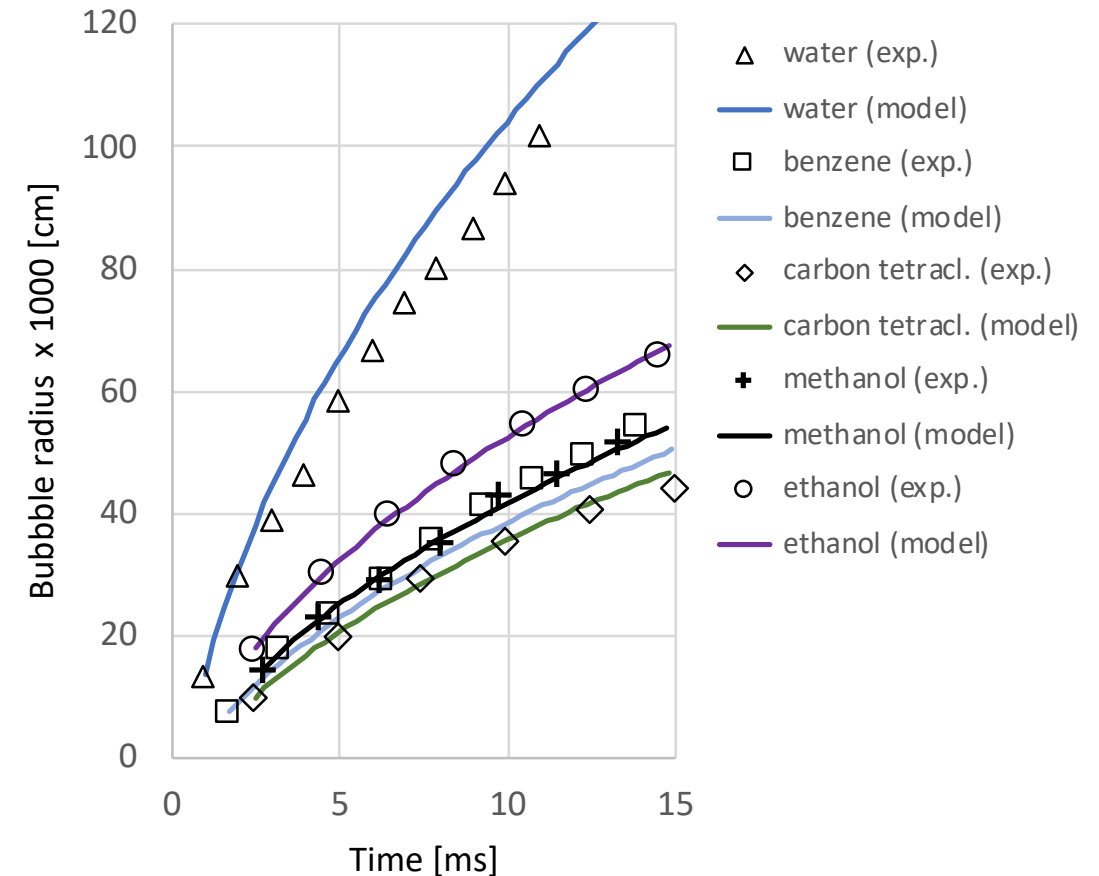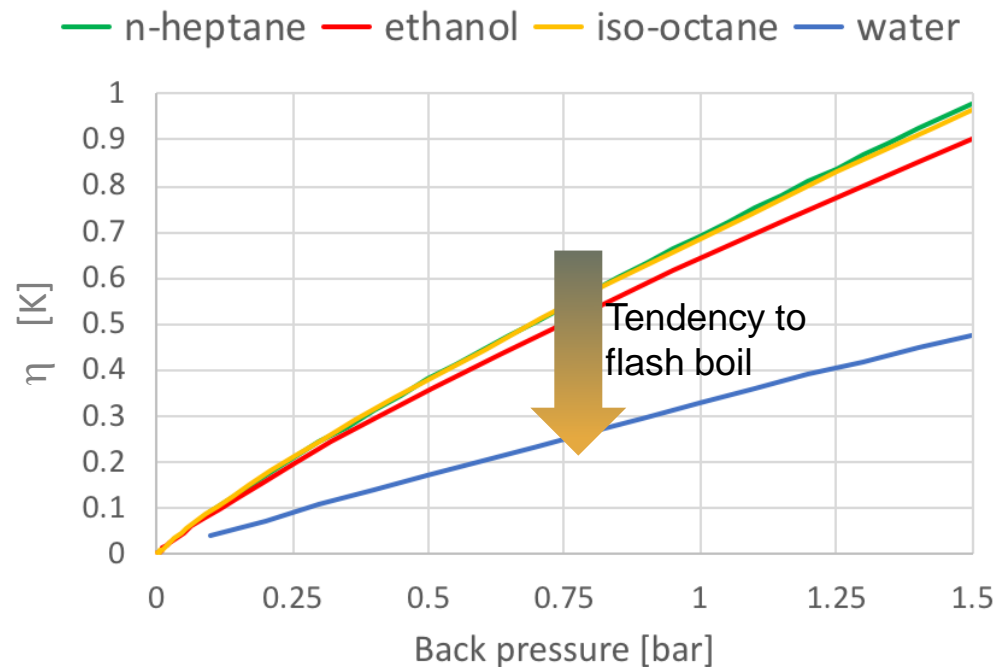$$\dot{m} = \frac{[\mathbf{n}_\Gamma \cdot \nabla T]_\Gamma}{[h]}$$

Sensitivity of flash boiling to fuel properties

$$\text{Ja} \cdot \frac{\rho_{vap}}{\rho_{liq}} = \frac{\rho_{vap}}{\rho_{liq}} \cdot \frac{c_{p,liq}}{h_{vap}} \cdot \Delta T_0 = \frac{\Delta T_0}{\eta}$$

— n-heptane — ethanol — iso-octane — water

Tendency to flash boil

Bubble radii as a function of time in various superheated liquids (symbols) compared to growth model predictions (lines)
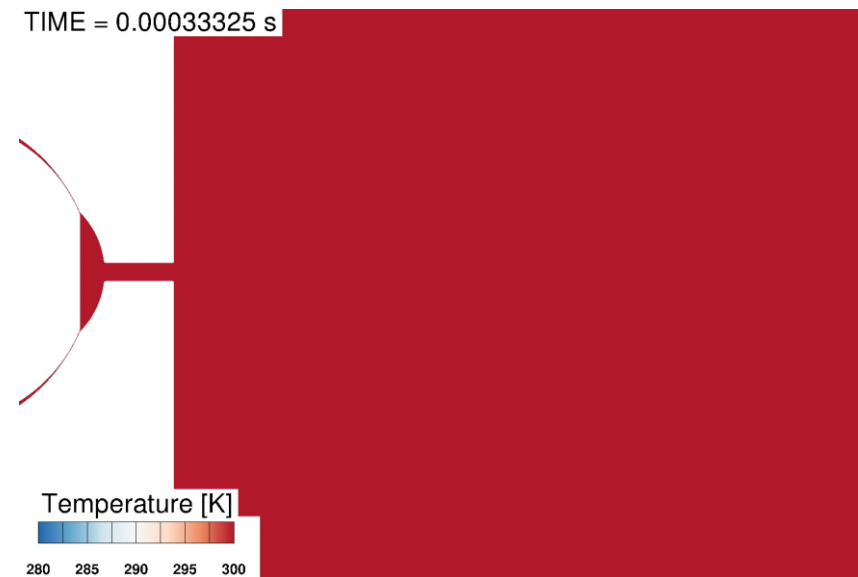
Note difference in mixture temperature and vapor angle

Current Θ_{HRM} implementation

NEW: $\Theta_{HRM}(Ja)$

Lines: Y_{C5H12} = 0.02, 0.08
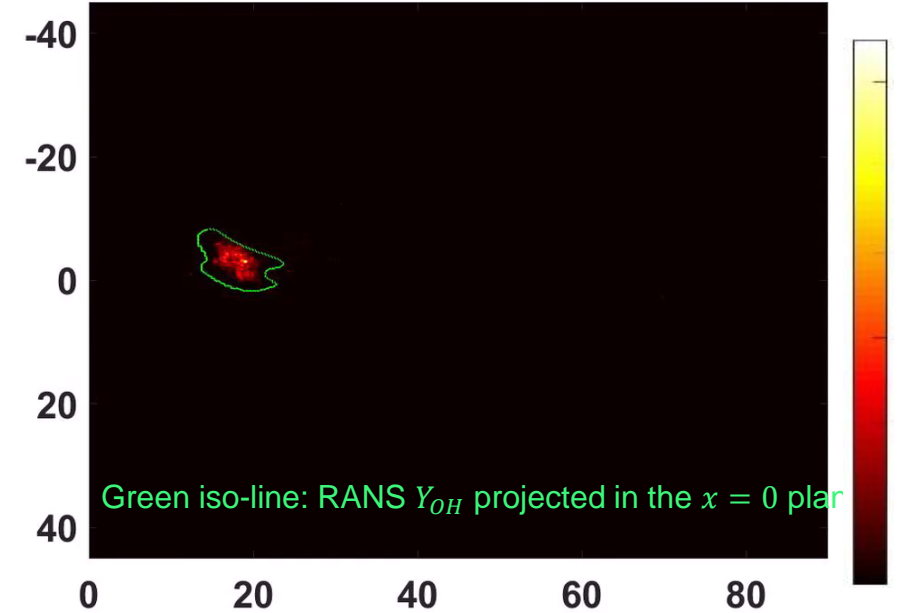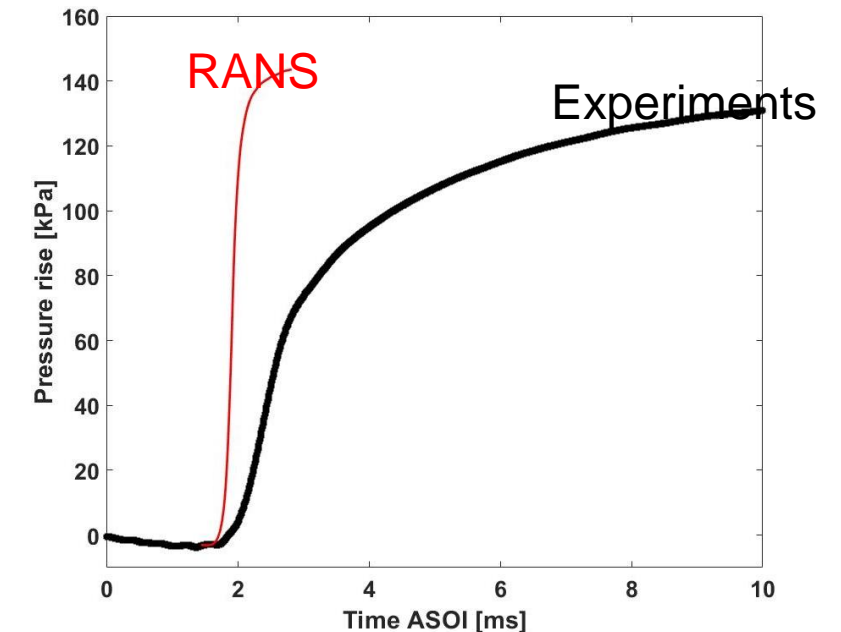
Iso-lines:

$z_{st} = 0.061$

$T = 1000\ K$

$Y_{OH} = 0.001$

Time =0.00144 s

Z

0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.13
0.11
0.09
0.07
0.05
0.03
0.01
0

Comparison OH* Expe / OH Converge at 1720us

Green iso-line: RANS Y_{OH} projected in the $x = 0$ plane

OH* experiments (averaged image)

RANS

Experiments

Several simulations have been performed varying the chemical mechanism, the ignition location and timing. They all present the same characteristics:

- The radial expansion of OH is greatly overestimated
- The flame propagates too fast, especially at the jet periphery

- **Combined high-speed OH and planar formaldehyde diagnostic shows position of early cool flame, high-temperature ignition, consumption of formaldehyde, and soot-free combustion with dilution (15% O_2) to limit NOx formation**

- **Ignition delays in sprays (stratified mixture and temperature) are slightly faster than well-stirred reactor calculations**

  - Is transport of cool-flame LTHR radicals a key reason for this behavior?

  - Sandia experiments repeat the ignition delay measurements made by CMT in a heated flow chamber at the same ECN conditions
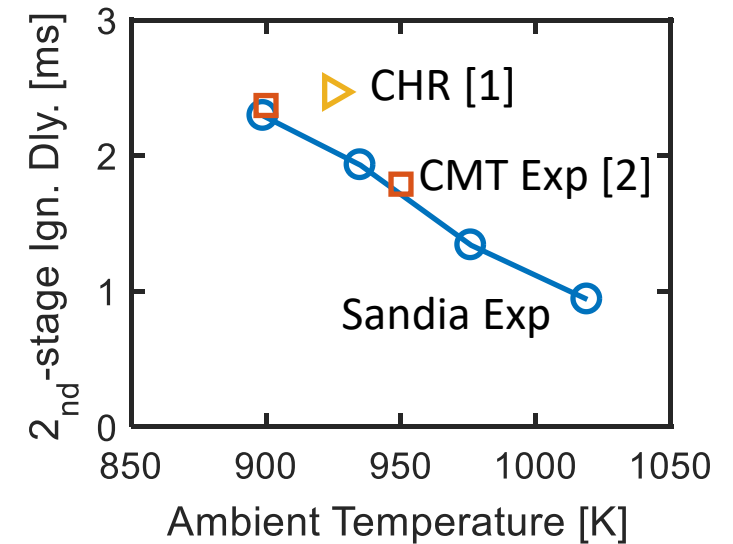
1. LLNL PRF mechanism 2004. Closed homogeneous reactor calculations at stoichiometric, adiabatic mixing condition from the ambient gas and fuel conditions
2. Pastor et al. Fuel 2016, ECN Spray A experiments in heated flow chamber
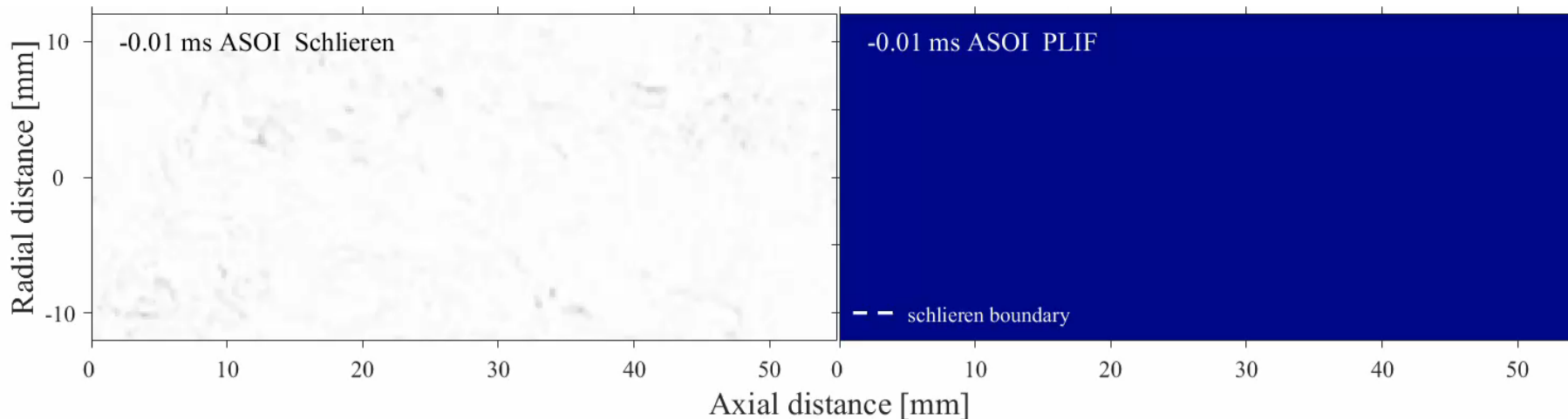
Fuel	PRF80
Ambient P [bar]	67
Ambient T [K]	1020
Amb. density [kg/m³]	22.8
Oxygen [mol%]	15
Injector	ECN Spray A-3